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FILE 'CAPLUS' ENTERED AT 15:55:33 ON 11 JUL 2003

L1 0 SEA ABB=ON PLU=ON CORN (S) (NIR (4A) SPECTR?) (S) "WET
CHEMISTRY"

L2 23 SEA ABB=ON PLU=ON CORN? (S) (NIR (4A) SPECTR?)

D L2 TI 1-23

D L2 IBIB ABS 1-23

L3 1 SEA ABB=ON PLU=ON CORN? (S) (NIR OR "NEAR-IFRARED" OR
INFRARED) (S) (WET (2A) CHEM?)

D L3 IBIB ABS

> d l2 ibib abs 1-23

L2 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2003:246661 CAPLUS

DOCUMENT NUMBER: 138:400627

TITLE: Dual-domain regression analysis for spectral calibration models

AUTHOR(S): Tan, Huwei; Brown, Steven D.

CORPORATE SOURCE: Department of Chemistry and Biochemistry, Brown
Laboratory, University of Delaware, Newark, DE, 19716, USA

SOURCE: Journal of Chemometrics (2003), 17(2), 111-122

CODEN: JOCHEU; ISSN: 0886-9383

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Taking advantage of the local nature of spectral data in both the time and frequency domains, two novel chemometric algorithms using the wavelet transform, namely dual-domain partial least squares (DDPLS) and dual-domain principal component regression (DDPCR), are reported here. The proposed algorithms establish parallel, regular models to describe spectral variation in the time (wavelength) domain. They incorporate these parallel models as a way of emphasizing local features in the frequency domain. Compared with regular PLS or PCR regression models applied to a single domain, these algorithms generate more parsimonious regression models that are also more robust against unexpected variations in the prediction set. Simulation data have been used in this paper to demonstrate this improvement. The new methods have also been successfully applied to NIR spectral data sets to predict moisture, oil, protein and starch content in Cargill corn samples, as well as a set of properties in a series of Amoco hydrocarbon samples. Through their special emphasis on the local nature of spectral signals in the frequency domain, spectral variance can be sep. explained over the frequency and time domains with fewer latent variables and with better predictive performance.

REFERENCE COUNT: 13

L2 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2003:125281 CAPLUS

DOCUMENT NUMBER: 139:35268

TITLE: Prediction of chemical composition, nutritive value and ingredient composition of European compound feeds for rabbits by near infrared reflectance spectroscopy (NIRS)

AUTHOR(S): Xiccato, G.; Trocino, Angela; De Boever, J. L.; Maertens, L.; Carabano, Rosa; Pascual, J. J.; Perez, J. M.; Gidenne, T.; Falcao-E-Cunha, Luisa

CORPORATE SOURCE: Dipartimento di Scienze Zootecniche, Agripolis, Universita degli Studi di Padova, Legnaro, I-35020, Italy

SOURCE: Animal Feed Science and Technology (2003), 104(1-4), 153-168

CODEN: AFSTDH; ISSN: 0377-8401

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Near IR reflectance spectroscopy (NIRS) was used to predict the chem. constituents, digestibility and energy value of 164 exptl. compd. feeds for rabbits using harmonized methods in 6 European institutes. NIRS equations were developed by partial least square regression (PLSR) using two-thirds of the samples as a calibration set and the remaining samples as a validation set. Prediction was satisfactory for the following characteristics: dry matter (coeff. of detn. in validation, $R^2=0.70$; std. error of prediction, $SEP=4.8$ g kg⁻¹), crude protein ($R^2=0.86$; $SEP=5.6$ g kg⁻¹ DM), ether ext. ($R^2=0.93$; $SEP=4.2$ g kg⁻¹ DM), ADF ($R^2=0.82$; $SEP=14$ g kg⁻¹ DM), starch ($R^2=0.90$; $SEP=16$ g kg⁻¹ DM), DM digestibility ($R^2=0.79$; $SEP=0.019$), gross energy digestibility ($R^2=0.81$; $SEP=0.019$) and digestible energy ($R^2=0.77$; $SEP=0.39$ MJ kg⁻¹ DM). NIRS prediction was less accurate for crude fiber ($R^2=0.60$; $SEP=16$ g kg⁻¹ DM), NDF ($R^2=0.50$; $SEP=32$ g kg⁻¹ DM), gross energy ($R^2=0.57$; $SEP=0.25$ MJ kg⁻¹ DM), while poor results were obtained for org. matter ($R^2=0.25$; $SEP=8.6$ g kg⁻¹ DM), ADL ($R^2=0.59$; $SEP=11$ g kg⁻¹ DM) and crude protein digestibility ($R^2=0.44$; $SEP=0.026$). The prediction of the inclusion rate of the main ingredients provided approx. indications on the feed formula. In particular, the prediction was good for the inclusion level of added fat ($R^2=0.87$), moderate for alfalfa meal (0.73), dried beet pulp (0.69), sunflower meal (0.68), wheat bran (0.66) and whole soya bean (0.63), but was poor ($R^2<0.50$) for grains (barley, wheat) and wheat straw. Grouping similar ingredients (starch concs., protein concs., wheat byproducts) slightly improved the prediction of the inclusion rate.

REFERENCE COUNT: 35

L2 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:887368 CAPLUS

DOCUMENT NUMBER: 138:38298

TITLE: Monitoring PV in corn and soybean oils by NIR spectroscopy

AUTHOR(S): Yildiz, Gulgun; Wehling, Randy L.; Cuppett, Susan L.

CORPORATE SOURCE: Department of Food Science and Technology, University of Nebraska, Lincoln, NE, 68583-0919, USA

SOURCE: Journal of the American Oil Chemists' Society (2002), 79(11), 1085-1089

CODEN: JAOCA7; ISSN: 0003-021X

PUBLISHER: AOCS Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB NIR spectroscopy was used successfully in our lab. to monitor oxidn. levels in vegetable oils. Calibration models were developed to measure PV in both soy and corn oils, using partial least squares (PLS) regression and forward stepwise multiple linear regression, from NIR transmission spectra. PV can be measured successfully in both corn and soy oils using a single calibration. The most successful calibration was based on PLS regression of first deriv. spectra. When this calibration was applied to validation sample sets contg. equal nos. of corn and soy oil samples, with PV ranging from 0 to 20 meq/kg, a correlation coeff. of 0.99 between titrn. and NIR values was obtained, with a std. error of prediction equal to 0.72 meq/kg. For both types of oil, changes occurred in the 2068 nm region of the NIR spectra as oxidn. levels increased. These changes appear to be assocd. with the formation of hydroperoxides during oxidn. of the oils.

REFERENCE COUNT: 14

L2 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:424644 CAPLUS

DOCUMENT NUMBER: 137:62334

TITLE: "Near-Infrared Reflectance Spectroscopy (NIRS) Enables the Fast and Accurate Prediction of Essential Amino Acid Contents. 2. Results for Wheat, Barley, Corn, Triticale, Wheat Bran/Middlings, Rice Bran, and Sorghum"

AUTHOR(S): *Fontaine, Johannes; Schirmer, Barbara; Hoerr, Jutta*

CORPORATE SOURCE: Feed Additives Division Applied Technology, Degussa AG, Hanau, D-63403, Germany

SOURCE: **Journal of Agricultural and Food Chemistry (2002), 50(14), 3902-3911**

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Further NIRS calibrations were developed for the accurate and fast prediction of the total contents of methionine, cystine, lysine, threonine, tryptophan, and other essential amino acids, protein, and moisture in the most important cereals and brans or middlings for animal feed prodn. More than 1100 samples of global origin collected over five years were analyzed for amino acids following the Official Methods of the United States and European Union. Detailed data and graphics are given to characterize the obtained calibration equations. NIRS was validated with 98 independent samples for wheat and 78 samples for corn and compared to amino acid predictions using linear crude protein regression equations. With a few exceptions, validation showed that 70-98% of the amino acid variance in the samples could be explained using NIRS. Esp. for lysine and methionine, the most limiting amino acids for farm animals, NIRS can predict contents in cereals much better than crude protein regressions. Through low cost and high speed of anal. NIRS enables the amino acid anal. of many samples in order to improve the accuracy of feed formulation and obtain better quality and lower prodn. costs.

REFERENCE COUNT: 24

L2 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:132774 CAPLUS

DOCUMENT NUMBER: 137:62350

TITLE: Determination of the degree of gelatinisation of starch by near infrared spectroscopy

AUTHOR(S): Nzabonimpa, R.; Nicod, P.

CORPORATE SOURCE: Nestle Research Center, Lausanne, CH-1000/26, Switz.

SOURCE: Near Infrared Spectroscopy, Proceedings of the International Conference, 9th, Verona, Italy, June 13-18, 1999 (2000), Meeting Date 1999, 75-80. Editor(s): Davies, Anthony M. C.; Giangiacomo, Roberto. NIR Publications: Chichester, UK.

CODEN: 69CGZM; ISBN: 0-9528666-1-7

DOCUMENT TYPE: Conference

LANGUAGE: English

AB The degree of gelatinization of starch is calcd. by dividing the amt. of gelatinized starch by the amt. of total starch. The gelatinized starch is the amt. of glucose produced by the action of amyloglucosidase on the starch. The total starch is the amt. of glucose produced by the combined action of amylase and amyloglucosidase on the starch. Results of enzymic digestion calcn. for starch samples from corn flours, extruded flours, oat flours, rice semolina, tapioca, and wheat bran were compared to NIR spectroscopic measurements of the flour samples. Results indicated that a good correlation was obtained between the degree of gelatinization detd. by the enzymic method and NIR with a coeff. of detn. (R^2) of 0.988 and a std. error of calibration (SEC) of 2.27.

REFERENCE COUNT: 11

L2 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:91958 CAPLUS

DOCUMENT NUMBER: 137:32205

TITLE: Studies on near infrared reflectance spectroscopy (NIRS) analysis of corn for silage

AUTHOR(S): Lee, H. W.; Park, H. S.; Kim, J. D.

CORPORATE SOURCE: Dep. Agricultural Sci., Korea National Open Univ., S. Korea

SOURCE: Journal of Animal Science and Technology (2001), 43(6), 981-988

CODEN: JASTCC

PUBLISHER: Korean Society of Animal Sciences and Technology

DOCUMENT TYPE: Journal

LANGUAGE: Korean

AB Dried finely chopped samples ($n=96$) were scanned at 2nm intervals over the wavelength range 400-2500nm and the optical data recorded as $\log 1/\text{Reflectance}(\log 1/R)$. Modified partial least squares(MPLS) regression was applied to scatter-cor. spectra (SNV and detrend). Calibration models for near-IR reflectance spectroscopy (NIRS) measurements gave multivariate correlation coeffs. of detn. (R^2) and std. errors of calibration (SEC) of 0.84(SEC 0.28), 0.94(SEC 1.74), 0.91(SEC 0.74) and 0.95(SEC 0.14) for content of dry matter(DM), neutral detergent fiber (NDF), acid detergent fiber (ADF) and crude protein (CP) on a dry basis resp. The std. error of prediction (SEP) on the validation set ($n=36$) was used in comparisons of prediction accuracy. The SEP value

was 0.33(DM), 1.79(NDF), 0.7(ADF) and 0.1%(CP), resp. The relative ability of NIRS to predict chem. compn. was very good for CP, NDF and ADF, and low for DM. This research should be useful in the rapid anal. of forage quality for research and the industry.

L2 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:505590 CAPLUS

DOCUMENT NUMBER: 135:272051

TITLE: Network of VDLUFA for the research of silage -experience from the years 1999 and 2000

AUTHOR(S): Tillmann, P.; Dieterle, P.; Engling, F.-P.; Horst, H.

CORPORATE SOURCE: VDLUFA, Kassel, D-34128, Germany

SOURCE: VDLUFA-Schriftenreihe (2000), 55, 4-8

CODEN: VDSCEE; ISSN: 0173-8712

PUBLISHER: VDLUFA-Verlag

DOCUMENT TYPE: Journal

LANGUAGE: German

AB Near-IR spectroscopy (NIRS) network calibrations were established for the detn. of the quality of grass and corn silages of any origin with high precision. Calibrations were established for the markers dry matter, raw protein, raw fiber, raw fat, ADF, and NDF as well as reducing sugars and gas formation for grass silage and raw starch and eulos for corn silages. A good precision was confirmed in ring examns. and validations.

REFERENCE COUNT: 12

L2 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:426522 CAPLUS

DOCUMENT NUMBER: 135:179840

TITLE: Determination of the total unsaturation in vegetable oils by Fourier transform Raman spectroscopy and multivariate calibration

AUTHOR(S): Barthus, R. C.; Poppi, R. J.

CORPORATE SOURCE: Instituto de Quimica, Universidade Estadual de Campinas, Campinas, SP, 13083-970, Brazil

SOURCE: Vibrational Spectroscopy (2001), 26(1), 99-105

CODEN: VISPEK; ISSN: 0924-2031

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In this paper multivariate calibration was used in conjunction with NIR-Fourier transform Raman spectroscopy for detn. of the total degree of unsatn. in vegetable oils. For this purpose, different vegetable oils and some mixts. were employed as calibration stds. A calibration model based on partial least squares (PLS) was constructed and used to analyze oils with iodine values ranging from 17 to 130. This methodol. is rapid, simple and can be easily used in quality control labs. or to monitor industrial process on line.

REFERENCE COUNT: 9

L2 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:197185 CAPLUS

TITLE: Monitoring oxidation in vegetable oils by near-IR spectroscopy

AUTHOR(S): Wehling, Randy L.; Yildiz, Gulgun; Cuppett, Susan L.

CORPORATE SOURCE: Department of Food Science and Technology, University of Nebraska, Lincoln, NE, 68583-0919, USA

SOURCE: Abstracts of Papers - American Chemical Society (2001), 221st, ANYL-099

CODEN: ACSRAL; ISSN: 0065-7727

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal; Meeting Abstract

LANGUAGE: English

AB Near-IR (NIR) spectroscopy has been used successfully in our lab. to monitor oxidn. levels in vegetable oils. Models have been developed to measure peroxide values in both soy and corn oil, using Partial Least Squares (PLS) regression and Multiple Linear Regression (MLR), from NIR transmission spectra. Peroxide values can be successfully measured in both corn and soy oil using a single model. The most successful model was based on PLS regression of first deriv. spectra. When this model was applied to validation sample sets contg. equal nos. of corn and soy oil samples, with peroxide values ranging from 0-20 meq/kg, a correlation coeff. of 0.99 between titrn. and NIR values was obtained, with a std. error of prediction (SEP) equal to 0.72 meq/kg. For both types of oil, changes occurred in the 2068 nm region of the NIR spectra as oxidn. levels increased. These changes appear to be assocd. with the formation of hydroperoxides during oxidn. of the oils.

L2 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:114287 CAPLUS

DOCUMENT NUMBER: 132:250183

TITLE: Predicting protein content by near infrared reflectance spectroscopy in diverse cereal food products

AUTHOR(S): Kays, Sandra E.; Barton, Franklin E., II; Windham, William R.

CORPORATE SOURCE: Agricultural Research Service, Richard B. Russell Agricultural Research Center, US Department of Agriculture, Athens, GA, 30604-5677, USA

SOURCE: Journal of Near Infrared Spectroscopy (2000), 8(1), 35-43

CODEN: JNISEI; ISSN: 0967-0335

PUBLISHER: NIR Publications

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Simultaneous detn. of constituents (e.g. dietary fiber, protein, fat) by near IR (NIR) spectroscopy would increase the speed and efficiency of nutrient anal. while substantially reducing the cost. Previous work has described the development of NIR reflectance models for the prediction of dietary fiber in a diverse group of cereal food products. While NIR spectroscopy has been used to measure protein content in cereal samples comprised of a single grain type, the utility of the NIR technique would be greatly improved if it could be expanded to cereal products derived from a diverse cross-section of grains and formulations. The present study was conducted to investigate the potential

of NIR spectroscopy for the anal. of protein in a data set that included products with numerous grains, such as wheat, oats, rice, rye, corn, millet, buckwheat and with a wide range of fat, sugar and fiber contents. In addn., numerous processing techniques and food additives were represented in the data set. Nitrogen content of dry-milled cereal products was measured by combustion anal. (AOAC Method 992.23) and the range in nitrogen values was from 0.65 to 3.31% of dry wt. Milled cereal products were scanned from 1100 to 2500 nm with a scanning monochromator. A nitrogen calibration was developed, using a com. anal. program, with modified partial least squares as the regression method. The std. error of cross validation and R² for nitrogen (n=147 calibration samples) were 0.090% and 0.973, resp. Independent validation samples (n=72) were predicted with a std. error of performance of 0.079% nitrogen and r² of 0.984. Because of the diversity of grains in the data set, crude protein was calcd. using two nitrogen-to-protein conversion methods and two PLS models were developed for the prediction of crude protein. Crude protein was predicted with a similar precision to nitrogen and the results for both protein models are within the precision required for US nutrition labeling legislation. In conclusion, NIR reflectance spectroscopy can be used for rapid and accurate prediction of nitrogen and crude protein in a heterogeneous group of cereal products comprised of a wide cross-section of grains and formulations.

REFERENCE COUNT: 25

L2 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:760996 CAPLUS

DOCUMENT NUMBER: 132:83752

TITLE: Corn starch identification by near infrared spectroscopy

AUTHOR(S): Hackmann, Erika Rosa Maria Kedor; De Abreu, Esmeralda Maria Cupello; Santoro, Maria Ines Rocha Miritello

CORPORATE SOURCE: Departamento de Farmacia, Faculdade de Ciencias Farmaceuticas, Universidade de Sao Paulo, Sao Paulo, SP, 05389-970, Brazil

SOURCE: Revista Brasileira de Ciencias Farmaceuticas (1999), 35(1), 141-146

CODEN: RBCFFM; ISSN: 1516-9332

PUBLISHER: Universidade de Sao Paulo, Faculdade de Ciencias Farmaceuticas

DOCUMENT TYPE: Journal

LANGUAGE: Portuguese

AB Near IR spectroscopy (NIR) was used to identify corn starch in pharmaceutical raw materials and products. A NIR spectral library (1100-2500 nm) was created and used as a ref. for the anal. of raw drug materials. The library were obtained using data from 5 different corn starch batches that were first analyzed by official methods. Later 17 new corn starch spectra were added to the original library to improve the data variability. Two spectral parameters used during the library calibration were distance and correlation processed by the software NSAS module IQ2. NIR spectroscopy method is fast, cost-efficient, and suitable for quality control systems.

REFERENCE COUNT: 10

L2 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:584495 CAPLUS

DOCUMENT NUMBER: 131:269158

TITLE: Feasibility of Rapid and Nondestructive Determination of Ash Content in Cornu Cervi Parvum Using Near-Infrared Spectroscopy

AUTHOR(S): Woo, Young-Ah; Kim, Hyo-Jin; Park, Sang-Yong; Chang, Seung-Yeup; Chung, Hoeil

CORPORATE SOURCE: College of Pharmacy, Dongduk Women's University, Seoul, 136-814, S. Korea

SOURCE: Microchemical Journal (1999), 63(1), 154-160

CODEN: MICJAN; ISSN: 0026-265X

PUBLISHER: Academic Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Near-IR (NIR) spectroscopy was applied to the nondestructive and rapid detn. of ash content in Cornu Cervi Parvum, a dried horn of Cervus nippon or Cervus elaphus, which serves as a natural drug for general health care in Asian countries. Cervine horns are dried for use as a drug and are classified according to their age as either Cornu Cervi Parvum (new horn) or Cervi Cornu (old horn). Ash content is generally used to det. the quality of cervine horns. A traditional method to det. ash content is an ignition method that measures ash residue after incineration. However, >4 h is required for incineration and the destruction of org. compds. NIR spectroscopy was studied as an alternative anal. method to decrease anal. time and increase lab. efficiency. Using partial least-squares regression, relevant information related to ash in the NIR region was successfully extd. NIR prediction results showed good correlation with those from the ignition method. The overall results showed the feasibility of NIR spectroscopy for the detn. of ash content in Cornu Cervi Parvum. (c) 1999 Academic Press.

REFERENCE COUNT: 8

L2 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:619237 CAPLUS

TITLE: Study on determination of contents of oil in integrated kernel of corn using diffuse reflectance spectroscopy

AUTHOR(S): Zhang, Yehui; Longlian, Zhao; Song, Tongming; Yan, Yanlu

CORPORATE SOURCE: China Agricultural University, Beijing, 100094, Peop. Rep. China

SOURCE: Guangpuxue Yu Guangpu Fenxi (1998), 18(4, Spec.Issue), 99-100

CODEN: GYG FED; ISSN: 1000-0593

PUBLISHER: Beijing Daxue Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB This work is on researching method of determing contents of oil in an integrated kernel of corn using FT-NIR diffuse reflectance spectroscopy. Result shows that method is better for determing contents oil and correlation coeff. is 0.93 and relative error is near 10%. It suggests that method can be used in qual. breeding program.

L2 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:172792 CAPLUS

DOCUMENT NUMBER: 128:153246

TITLE: Prediction of Total Dietary Fiber by Near-Infrared Reflectance Spectroscopy in High-Fat- and High-Sugar-Containing Cereal Products

AUTHOR(S): Kays, Sandra E.; Windham, W. R.; Barton, Franklin E., II

CORPORATE SOURCE: Richard B. Russell Agricultural Research Center

Agricultural Research Service, U.S. Department of Agriculture, Athens, GA, 30604-5677, USA

SOURCE: Journal of Agricultural and Food Chemistry (1998), 46(3), 854-861

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The near-IR (NIR) spectral properties of cereal products contg. high fat or high sugar can differ substantially from the spectral properties of other cereal products. An existing NIR model, using preprocessed reflectance spectra and partial least-squares anal., for the prediction of total dietary fiber in cereal products was expanded to two new models called (1) the "fat-expanded" model and (2) the "fat- and sugar-expanded" model. The fat-expanded model enlarges the existing model with high-fat-content products as calibration samples, and the "fat- and sugar- expanded" model also includes products with high sugar and high cryst. sugar content. The dry milled cereal and grain products were analyzed in the lab. according to AOAC method 991.43 for the detn. of total dietary fiber, and NIR reflectance spectra were collected with a scanning monochromator. Data anal. and selection of representative high-fat and high-sugar samples were performed with a com. anal. program. The two expanded models had std. errors of cross-validation and R² similar to those of the existing model, with acceptable std. error of performance and r² when tested with independent validation samples. The existing model was, thus, expanded to include high-fat, high-sugar, and high cryst. sugar cereal products while maintaining prediction accuracy.

L2 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:104260 CAPLUS

DOCUMENT NUMBER: 128:191858

TITLE: Raman and NIR spectroscopic methods for determination of total dietary fiber in cereal foods: a comparative study

AUTHOR(S): Archibald, D. D.; Kays, S. E.; Himmelsbach, D. S.; Barton, F. E., II

CORPORATE SOURCE: Quality Assessment Research Unit, Russell Research Center, USDA Agricultural Research Service, Athens, GA, 30604-5677, USA

SOURCE: Applied Spectroscopy (1998), 52(1), 22-31

CODEN: APSPA4; ISSN: 0003-7028

PUBLISHER: Society for Applied Spectroscopy

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Partial least-squares regression (PLSR) was used to generate three Raman and three near-IR reflectance (NIRR) models for the spectroscopic detn. of total dietary fiber (TDF) of a wide variety of cereal foods. To allow comparison of the spectral techniques, both analyses used the same sets of samples (n_{cal} = 63, n_{val} = 63). Six models were

optimized by full leave-one-out cross-validation (CV), including a smoothed, a first-, and a second-deriv. model for each spectral technique. Both kinds of raw spectral data required correction of interfering baseline and amplitude variations. Deriv. preprocessing generally reduced the no. of latent variables (LVs) for both spectral types and significantly reduced the CV error of the Raman models. The deriv. treatments enhanced the influence of select vibrational-bandwidth-sized features in the Raman data (64-84 cm⁻¹). The Savitzky-Golay deriv. calcn. method was better for the NIR data, while the gap-difference method was better for the Raman data, which had a higher level of baseline noise. Raman models required 6 to 9 latent variables while NIR models required 10 to 14 LVs. The root-mean-squared CV model errors were 2-2.3% TDF for all six models, and the three Raman models had root-mean-squared prediction errors (RMSEPs) in the range 2.8-3.2% TDF, with the best model being generated from second-deriv. data. First-deriv. data provided the best NIR model, and for all three NIR models the RMSEP spanned 2.4-2.9%. For some types of samples, it is suggested that the Raman method is limited by its sampling technique and could be improved with more densely packed, larger-area specimens. The regression vectors of the Raman models seem more easily interpretable than NIR models. Either spectral method appears capable of achieving an acceptable level of error; TDF ref. method precision was 0.68% TDF, while the product label information had an error of 2.8% TDF relative to the ref.

REFERENCE COUNT: 21

L2 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:560665 CAPLUS

DOCUMENT NUMBER: 127:245018

TITLE: Application of near-infrared reflectance spectrometry in the study of atopy. Part 1. Investigation of skin spectra

AUTHOR(S): Dreassi, E.; Ceramelli, G.; Fabbri, L.; Vocioni, F.; Bartalini, P.; Corti, P.

CORPORATE SOURCE: Department of Chemical and Pharmaceutical Technology, Siena University, Siena, 53100, Italy

SOURCE: Analyst (Cambridge, United Kingdom) (1997), 122(8), 767-770

CODEN: ANALAO; ISSN: 0003-2654

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB An investigation into the existence of spectral differences and differences in response in terms of water and lipid content between normal and atopic skin is described. Since NIR radiation penetrates complex structured matrixes down to a depth of 0.15-0.20 mm, it is evident that the method lends itself to spectral detection of skin components down to the deepest level. First the reproducibility of readings made with the instrument was tested and it was also checked whether the use of the probe caused changes in skin equil. due to occlusion. Anal. of the NIR spectra did not enable normal and atopic subjects to be distinguished unequivocally but provided important information on the use of NIR spectrometry in these subjects and insights into the stratum corneum. Although the responses of water and lipid structures could not be read directly from the spectra, it was possible to decomp. the global spectral information into

components by principal components anal. It was possible to observe a fraction of variance assocd. in different ways with water.

L2 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:333094 CAPLUS

DOCUMENT NUMBER: 127:64715

TITLE: "Whole grain amylose analysis in maize using near-infrared transmittance spectroscopy"

AUTHOR(S): Campbell, M. R.; Brumm, T. J.; Glover, D. V.

CORPORATE SOURCE: Purdue Univ., IN, USA

SOURCE: Cereal Chemistry (1997), 74(3), 300-303

CODEN: CECHAF; ISSN: 0009-0352

PUBLISHER: American Association of Cereal Chemists

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The development of genetically modified starches has relied on the use of maize (*Zea mays* L.) endosperm mutant alleles that alter starch structural and phys. properties. A rapid method for predicting amylose content would benefit breeders and com. handlers of specialty starch corn. For this reason, a study was conducted to investigate the use of near-IR transmittance spectroscopy (NITS) as a rapid and nondestructive technique for predicting grain amylose content (BAC) in maize. Many single- and double-mutant inbreds and hybrids were used to create a calibration set for the development of a predictive model using partial least squares anal.. A validation set composed of similar genetic material was used to test the prediction model. A coeff. of correlation (r) of 0.94 was obsd. between GAC values detd. colorimetrically and those predicted by NITS; however, the predicted values were assocd. with a large std. error of prediction ($SEP = 3.5$). Overall, NITS discriminated well among high amylose and waxy genotypes. The NITS calibration was used to det. levels of contamination by normal kernels in waxy and high-amylose (Amy VII) grain samples intended for wet milling. In both cases, a 5% contaminated sample could be detected from pure samples according to predicted NITS values.

L2 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1997:139107 CAPLUS

DOCUMENT NUMBER: 126:250306

TITLE: A rapid determination of maize powder mixed in soybean meal by near infrared spectroscopy

AUTHOR(S): Liu, Zhihua

CORPORATE SOURCE: Qinhuangdao Import Export Commodity Inspection Bureau, Qinhuangdao, 066002, Peop. Rep. China

SOURCE: Fenxi Shiyanshi (1996), 15(5), 84-88

CODEN: FENSE4; ISSN: 1000-0720

PUBLISHER: Beijing Daxue Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB Near-IR spectroscopy (NIR) anal. of soybean meal and the soybean meal mixed with some maize powder showed that the actual starch content in the soybean meal mixt. was correlated to the absorption bands at 2060, 2090 and 2166 nm. A linear regression equation was obtained by the regression anal., and the maize powder content of the soybean meal mixt. was calcd. by starch content in maize powder. A set of samples of soybean and maize powder mixts. was tested to det. the maize powder content, and the result showed the regression coeff. was 0.99.

L2 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:629659 CAPLUS

DOCUMENT NUMBER: 125:274187

TITLE: Prediction of corn dry-milling quality by near-infrared spectroscopy

AUTHOR(S): Wehling, R. L.; Jackson, D. S.; Hamaker, B. R.

CORPORATE SOURCE: Dep. of Food Sci. and Technology, Univ. of Nebraska, Lincoln, NE, 68583-0919, USA

SOURCE: Cereal Chemistry (1996), 73(5), 543-546

CODEN: CECHAF; ISSN: 0009-0352

PUBLISHER: American Association of Cereal Chemists

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The potential for near-IR (NIR) reflectance spectroscopy to predict corn dry-milling quality has been investigated. NIR spectra were obtained from samples of whole-kernel yellow dent corn. Dry-milling quality of the samples was evaluated with a Tangential Abrasive Dehulling Device (TADD), and by a short-flow lab. milling procedure that allowed calcn. of milling evaluation factor (MEF). Calibrations relating TADD index and MEF to NIR measurements were developed and tested with validation sample sets. The results indicate that NIR spectroscopy can predict dry-milling characteristics with a reliability suitable for at least rough screening. For MEF, the best calibration yielded a correlation coeff. of 0.90 and a std. error of prediction (SEP) of 1.55%. SEP values for TADD index were somewhat higher. Derivatization of the NIR spectra lowered the SEP values compared to the use of underivatized log 1/R measurements.

L2 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1994:268706 CAPLUS

DOCUMENT NUMBER: 120:268706

TITLE: Prediction of wet-milling starch yield from corn by near-infrared spectroscopy

AUTHOR(S): Wehling, R. L.; Jackson, D. S.; Hooper, D. G.; Ghaedian, A. R.

CORPORATE SOURCE: Dep. Food Sci. Technol., Univ. Nebraska, Lincoln, NE, 68583-0919, USA

SOURCE: Cereal Chemistry (1993), 70(6), 720-3

CODEN: CECHAF; ISSN: 0009-0352

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Near-IR reflectance (NIR) spectroscopy was used to predict the wet-milling starch yield obtainable from yellow dent corn. Spectral differences between samples with high and low starch yields were obsd. in two wavelength regions, 2,265-2,325 and 1,050-1,125

nm. The higher-wavelength region corresponds to known carbohydrate absorption bands; however, the origin of the shorter-wavelength differences is less clear. Different combinations of sample handling and spectral treatments were also evaluated, and the most successful instrument calibration used a multiterm linear equation of second-deriv. reflectance terms obtained from whole-kernel corn. Multiple correlation coeffs. for the various calibrations ranged from 0.8 to 0.9, with reproducibility of the lab. wet-milling procedure being a limiting factor. Application of the optimized calibration to a validation set contg. samples from two crop years gave a bias-cor. std. error of prediction equal to 1.41%, a result equal to or better than the std. error of the ref. method.

L2 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1994:243266 CAPLUS

DOCUMENT NUMBER: 120:243266

TITLE: Comparison of near-infrared spectroscopy and other soil nitrogen availability quick tests for corn

AUTHOR(S): Fox, Richard H.; Shenk, John S.; Piekielek, William P.; Westerhaus, Mark O.; Toth, John D.; Macneal, Kirsten E.

CORPORATE SOURCE: Dep. Agron., Pennsylvania State Univ., University Park, PA, 16802, USA

SOURCE: Agronomy Journal (1993), 85(5), 1049-53

CODEN: AGJOAT; ISSN: 0002-1962

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new quick test for soil N availability for corn using a near-IR spectrophotometer (NIRS) was compared with three published quick tests for predicting soil N-supplying capability (NSC) and relative corn grain yield. The other tests were the pre-sidedress nitrate test (PSNT), nitrate concn. (at-plant NO₃), and absorbance at 200 nm of a 0.01 M NaHCO₃ ext. (UV-200 test) of 0- to 20-cm soil samples taken at planting. Soil samples taken at planting from 95 field expts. in Pennsylvania were analyzed at reflectance wavelengths from 400 nm to 2500 nm with NIRS. The coeffs. of detn. were the same ($R^2 = 0.49$) for both linear and quadratic regressions of NSC and NIRS test values. The abilities of the four tests to predict NSC and relative corn grain yield were compared using data from 90 of the 95 expts. The R^2 values for linear and quadratic regressions between soil test values and NSC ranged from 0.49 to 0.58 for the NIRS, PSNT, and UV-200 tests; for the at-plant NO₃ test, R^2 was lower (.apprxeq.0.40). Eliminating sites where corn directly followed a legume, R^2 values for quadratic regressions between test values and NSC increased to .apprxeq.0.60 for the NIRS, PSNT, and UV-200 tests. The PSNT test was slightly better than the other tests in predicting a grain yield response to N fertilizer, but this advantage lessened when first-year-after-legume sites were eliminated. No test could accurately predict relative grain yield or NSC in fields responding to N fertilizer ($R^2 = 0.08-0.36$). The NIRS test offers a convenient, rapid, and inexpensive alternative to the PSNT for predicting whether humid-region corn fields will respond to N fertilizer.

L2 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1993:558501 CAPLUS

DOCUMENT NUMBER: 119:158501

TITLE: "Automated NIR analysis for routine feed evaluation"

AUTHOR(S): *Blank, F. T.; Vedder, H. W.*

CORPORATE SOURCE: BLGG, Oosterbeek, 6860 AC, Neth.

SOURCE: **Near Infra-Red Spectrosc. (1992), 197-202. Editor(s): Hildrum, Kjell Ivar. Horwood: Chichester, UK.**

CODEN: 59EBAF

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Corn samples were analyzed by near-IR spectrometry (NIRS) using a 2-part autosampler with an NIRSystems 6250 at .ltoreq.90 samples/h. Prediction of moisture, crude protein, and digestible org. matter was sufficiently accurate, whereas prediction of crude ash was poor in samples with high ash content. NIRS also could predict constituents needed for calcg. the feeding value of grass silages.

L2 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1985:503522 CAPLUS

DOCUMENT NUMBER: 103:103522

TITLE: The determination of fiber, starch, and total carbohydrate in snack foods by near-infrared reflectance spectroscopy

AUTHOR(S): Baker, Doris

CORPORATE SOURCE: Agric. Res. Serv., U.S. Dep. Agric., Beltsville, MD, USA

SOURCE: Cereal Foods World (1985), 30(6), 389-92

CODEN: CFWODA; ISSN: 0146-6283

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Near-IR reflectance (NIR) spectroscopy was used to det. fiber, starch [9005-25-8], and total carbohydrate in potato chips, corn chips, extruded snacks, popcorn, crackers, and pretzels. NIR predictions of fiber and starch were related to chem. anal. values as detd. by AACC method 32-20, Insol. Dietary Fiber, and a GLC method for starch. The sum of fiber and starch values is an est. of total carbohydrate in the types of foods in this study. The correlations of the NIR predictions to fiber, starch, and total carbohydrate, resp., were: 0.833 with std. error of 1.4% fiber, 0.946 with std. error of 3.5% starch, and 0.949 with std. error of 3.3% total carbohydrate.

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1987:495402 CAPLUS

DOCUMENT NUMBER: 107:95402

TITLE: "Use of near infrared reflectance spectroscopy in forage testing"

AUTHOR(S): *Jones, G. M.; Wade, Nancy S.; Baker, Judy P.; Ranck, Eugenie M.*

CORPORATE SOURCE: Dep. Dairy Sci., Virginia Polytech. Inst. and State Univ., Blacksburg, VA, 24061, USA

SOURCE: **Journal of Dairy Science (1987), 70(5), 1086-91**

CODEN: JDSCAE; ISSN: 0022-0302

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Near-IR reflectance spectroscopy anal. of forages for crude protein (CP), acid-detergent (ADF), and neutral-detergent (NDF) fiber and minerals was compared with wet chem. results. IR anal. was conducted with a NEO-Tech 51A where spectral equations had been transferred by the vendor from master calibrations. These calibrations were based upon microwave drying of feed samples and grinding through a cyclone mill. Forage was routinely tested by oven drying at 60.degree. and grinding with a Wiley mill through a 2-mm screen. Protein and ADF analyses were conducted on 66 corn silage, hay crop silage, and hay samples. Coeffs. of detn. for oven drying-wet chem. and microwave-IR, oven drying-wet chem. and oven drying-IR, and microwave-IR and oven drying-IR anal. were: 0.90, 0.93, and 0.98 for crude protein and 0.92, 0.94, and 0.96 for ADF. IR results were compared with wet chem. CP and ADF for 265 corn silage, hay, and hay crop silage samples. Coeffs. of detn. were 0.97 for CP and 0.94 for ADF with std. errors of prediction of 0.921 and 1.98. The resp. correlation coeffs. for corn silage, hay crop silage, and hay were 0.94 and 0.73; 0.95 and 0.92; and 0.73 and 0.74. Although std. errors of prediction were low for all minerals, coeffs. of detn. were above 0.80 for Ca and K.